1-Hexene

592-41-6 | DTXSID4025402

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -128 °C

Global applicability domain: Inside

Local applicability domain index: 9.76e-01

Confidence level: 8.90e-01

Nearest Neighbors from the Training Set

Image not found

1-Hexene
Measured: -140
Predicted: -128

Image not found

1-Heptene
Measured: -120
Predicted: -122

Image not found

2,4-Dimethylpent-2-ene
Measured: -128
Predicted: -122

Image not found

4-Methyl-2-pentene
Measured: -130
Predicted: -132